Combustion Simulations on the Cray XT3 at NCCS using S3D

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COMBUSTION RESEARCH FACILITY

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S3D project at NCCS

- S3D is a flow solver for performing direct numerical simulation (DNS) of turbulent combustion
  - S3D is a state-of-the-art code developed at CRF/Sandia
  - Has been ported and scales well on most office of science platforms
- Project title: “High-fidelity numerical simulations of turbulent combustion - fundamental science towards predictive models”
  - PI: Jacqueline H. Chen (SNL)
  - Past: ‘05 INCITE award, ‘05 and ‘06 LCF award
  - 2007 INCITE award (6M hours on XT3/4 at NCCS)

Direct Numerical Simulation (DNS)

Turbulent Combustion is a Grand Challenge

•Turbulent Combustion involves coupled phenomena at a wide range of scales.

- •Combustor size ~ 1m
- •Flame thickness 10~100μ

•O(10^4) continuum scales.

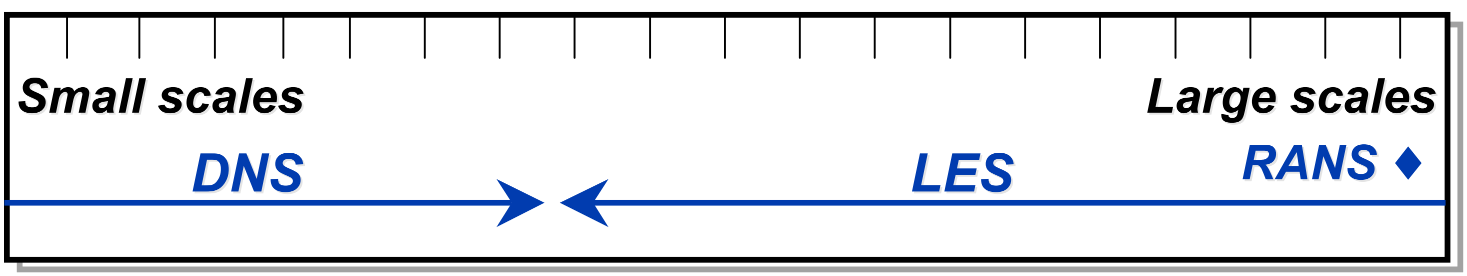
DNS Approach and Role

•Fully resolve all continuum scales without using sub-grid models

•Only a limited range of scales is computationally feasible.

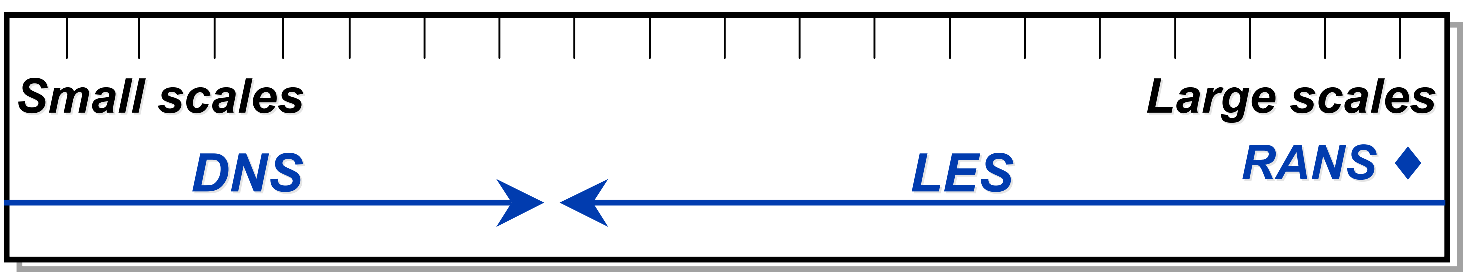
- •Terascale computing = DNS with O(10^3) scales for cold flow.

•DNS is limited to small domains. Device-scale simulations are out of reach.



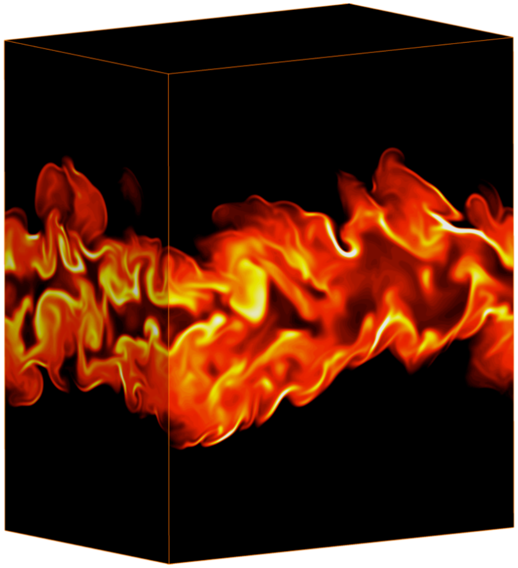
Example of Feasible Domain Size

- Grid spacing dictated by small scales of turbulence and chemistry
  - 15 ~ 30 microns necessary to fully resolve the reaction layer for typical flames
- 1 million grid points = 100 x 100 x 100
  - Domain size = 1.5 ~ 3mm
- 1 billion grid points = 1000 x 1000 x 1000
  - Domain size = 15 ~ 30mm
- Larger domain = wider range of scales
  - Closer to reality

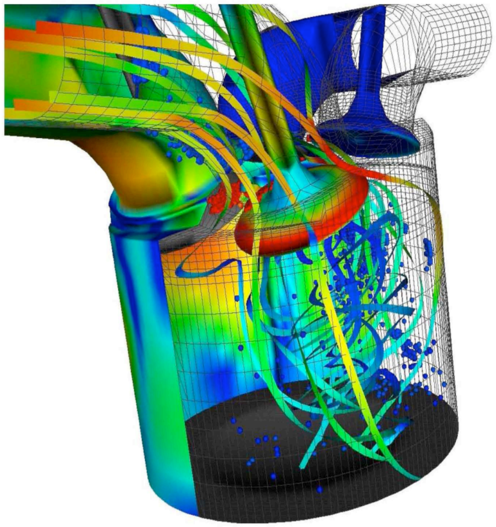


Role of Direct Numerical Simulation

- DNS is a tool for fundamental studies of the micro-physics of turbulent reacting flows
  - Full access to time resolved fields
  - Physical insight into chemistry turbulence interactions



- A tool for the development and validation of reduced model descriptions used in macro-scale simulations of engineering-level systems



DNS ↔ *Physical Models* ↔ *Engineering CFD codes (RANS, LES)*

S3D - DNS Solver

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S3D is a state-of-the-art DNS code developed at CRF/Sandia with 13 years of BES sponsorship.

- Solves compressible reacting Navier-Stokes equations.
- High fidelity numerical methods.
  - 8th order finite-difference
  - 4th order explicit RK integrator
- Hierarchy of molecular transport models
- Detailed chemistry
- Multi-physics (sprays, radiation and soot)
  - From SciDAC-TSTC (Terascale Simulation of Turbulent Combustion)
- Fortran90 and MPI
- Highly scalable and portable

S3D Optimization

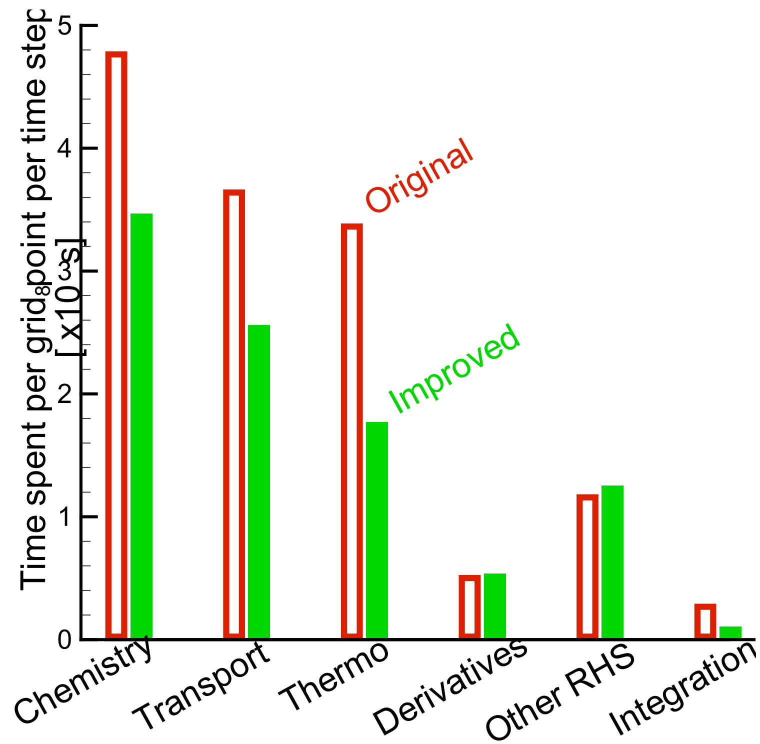
Scalar Optimizations

- Minimized CGS vs. SI unit conversions
- Tabulate and lookup thermodynamic properties
  - Previously computed using 7th degree polynomial
- Costs 45 % less

Vector Optimizations

- Vectorized chemistry, thermo and transport modules
- Vectorized nested loops
- 36 times faster

Profiling results from a 50^3 grid point 1-processor run



Scalar performance improvement

In collaboration with Mark Fahey (NCCS) and David Skinner (NERSC)

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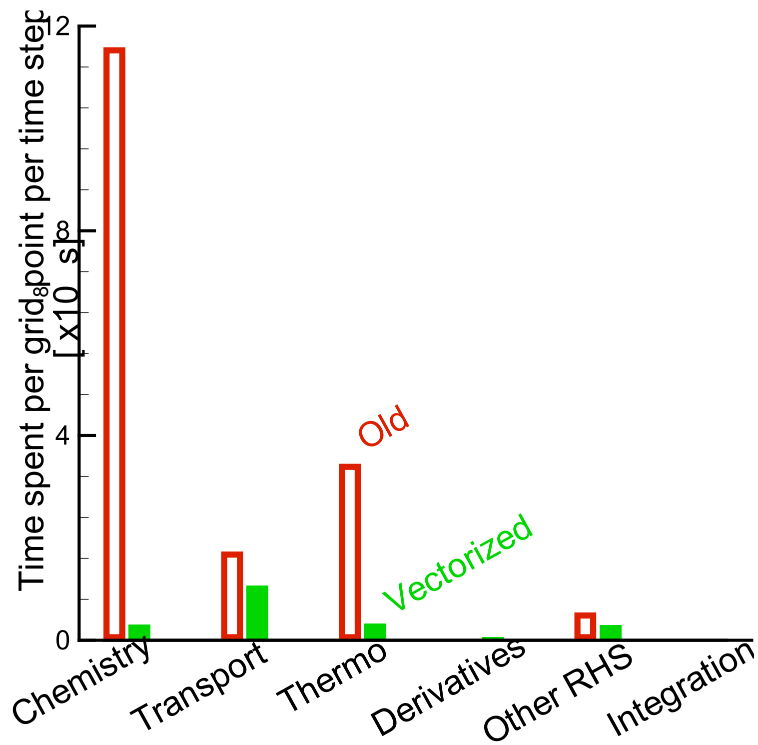

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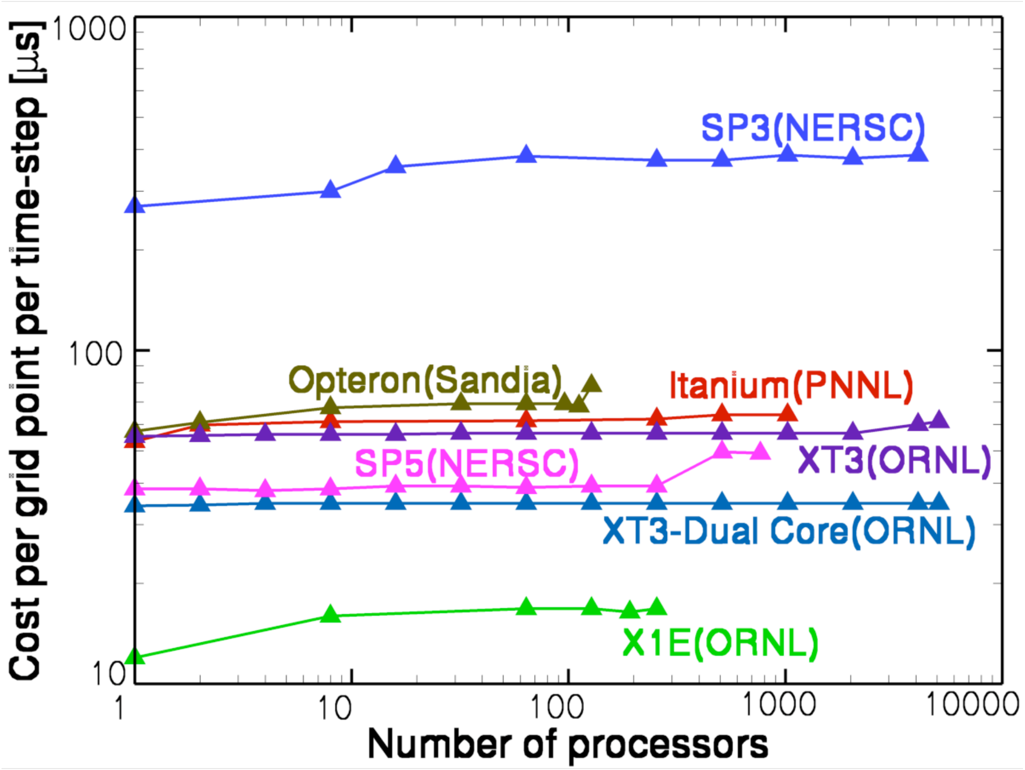
Parallelism

- Parallelism is achieved through 3D domain decomposition.
  - Each MPI process is in charge of a piece of the 3D domain.
- All MPI processes have the same number of grid points and computational load
- Inter-processor communication is only between nearest neighbors
  - Large message sizes. Non-blocking sends and receives
- All-to-all communications are only required for monitoring and synchronization ahead of I/O

$$\frac{\text{Communication}}{\text{Computation}} = \frac{kN^2}{kN^3} = \mathrm{O}\left(\frac{1}{\mathrm{N}}\right)$$

Parallel Performance and Improvements

- Eliminate MPI-derived data types for sending non-contiguous data
- Modified communication to reduce wait time
- Co-array communication



Multi-core performance

- How does S3D perform on multi-core processors?

S3D execution cost in (“core”-hours/gridpoint/timestep)x1e8 on XT4

	50^3 per core	40^3 per core	30^3 per core
yod -np 1 -SN	1.17	1.15	1.10
yod -np 2 -SN	1.17	1.15	1.10
yod -np 2 -VN	1.49	1.45	1.32

- Cost of executing the same problem is higher on a dual-core processor than a single-core processor.
  - craypat profile shows sections of code operating on large arrays went up in cost.
- The simulation turns around faster in wall-clock time when both cores of the dual-core processor are utilized.

I/O Strategy

- Restart data is also the analysis data
- Data written to disk ~ once per hour
- Each MPI thread writes to a separate file
- Unformatted fortran binary I/O
- Lustre stripe width set to 1. No striping.

3D DNS of a Spatially-Developing Turbulent Premixed Bunsen Flame

Performed on Cray X1E and XT3 at NCCS
’05 early user award and ’06 NLCF award

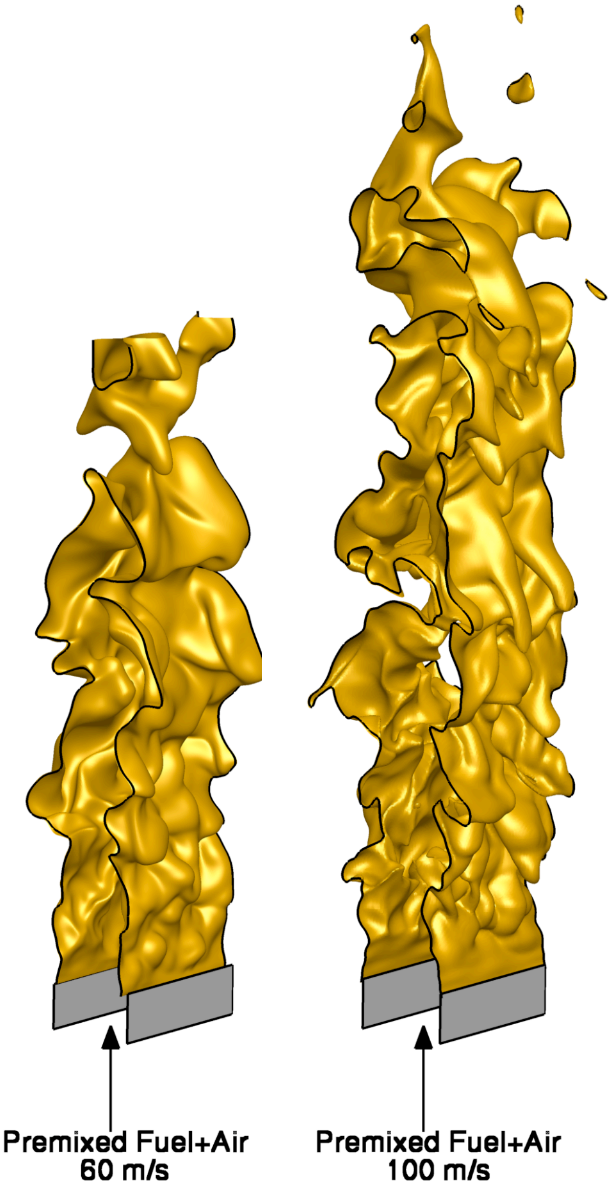
“Structure of a spatially developing turbulent lean methane-air bunsen flame”
By R. Sankaran, E. R. Hawkes, J. H. Chen, T. F. Lu and C. K. Law
in Proceedings of 31st combustion symposium (2006).

“Study of premixed flame thickness using
direct numerical simulation in a slot burner configuration”,
44th AIAA Aerospace Sciences Meeting, Paper No. 2006-0165

“Direct numerical simulation of stationary lean premixed
methane-air flames under intense turbulence ”,
5th US National Combustion Meeting, (2007).

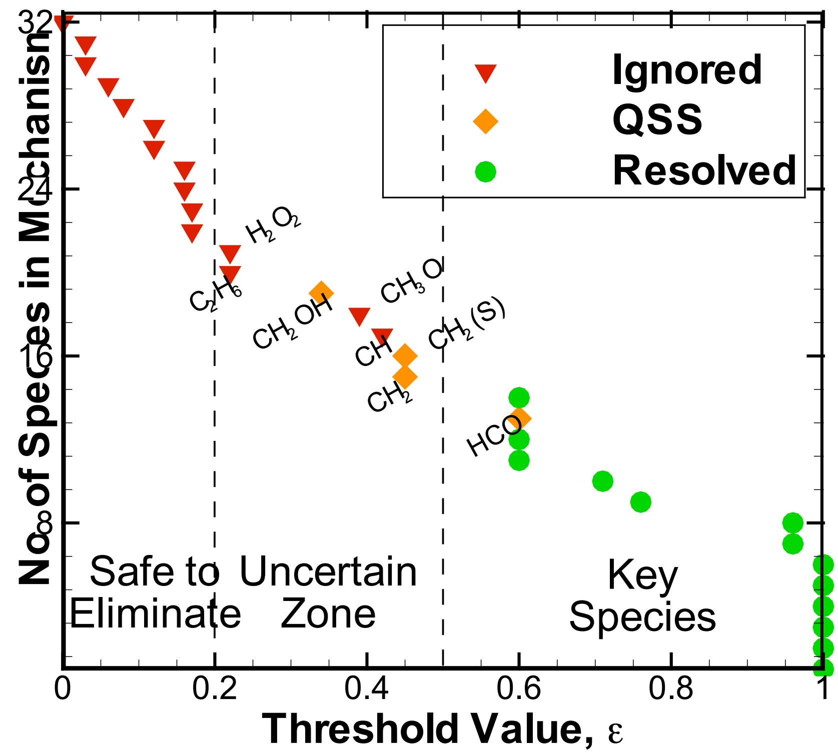
DNS of Lean Premixed Combustion

- **Goals**
  - Better understanding of lean premixed combustion in natural-gas based stationary gas turbines
  - Model validation and development
- **Simulation details**
  - Detailed CH_4/Air chemistry (18 D.O.F.)
  - Slot burner configuration with mean shear
  - Spatially developing and statistically stationary simulation.
    - Better suited for model development
  - A unique and first of its kind DNS.
  - Three different simulations at increasing turbulence intensities
    - To understand the effect of turbulent stirring on flame structure and burning speed.



Reduced Chemistry Model

- Usual CH_4-Air mechanisms are not suitable for DNS
- "Designer" reduced chemistry for DNS
  - By T. Lu and C.K. Law (Princeton)
- Starting with GRI1.2
  - 32 species, 177 reactions
- Identify species for elimination
  - Directed relation graph (DRG)
  - Sensitivity analysis
- Eliminate unimportant species
- Quasi-steady state assumption for CH_2OH, CH_2, $CH_2(s)$, HCO
  - Explicit algebraic relations
  - No costly iterations
  - Vectorization friendly



Simulation Parameters

	Case 1	Case 2	Case3
Jet Reynolds no. (Re_{jet})	840	1400	2100
Turbulence Reynolds no. (Re_t)	40	75	250
Karlovitz Number $(\delta_L/l_k)^2$	100	100	225
u'/S_L	3	6	10
Integral length scale (l_{33}/δ_L)	2	2	4
Number of Grid points	52M	88M	194M
Simulation performed on	X1E 512 MSPs	XT3 4800 cores	XT3 7200 cores

Flame speed (S_L)	1.8 m/s
Flame thicness based on maximum temperature gradient (δ_L)	0.3 mm
Nominal flame thickness (ν/S_L)	.05 mm
FWHM of heat-release layer (δ_H)	0.15 mm

Challenges in Data Analysis

- Large data sizes. 30TB of data generated last year.
- Analysis is an iterative process

<u>DNS Data</u>
Primitive scalars on original grid

↓

Obtain derived variables, fluid properties and their spatial derivatives

↓

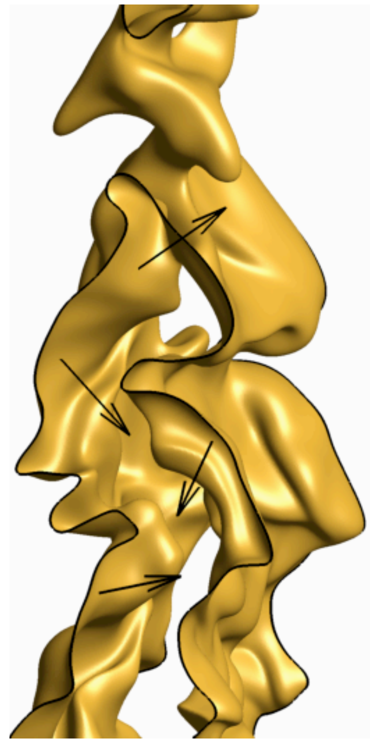
Identify flame features using primitive/derived variables

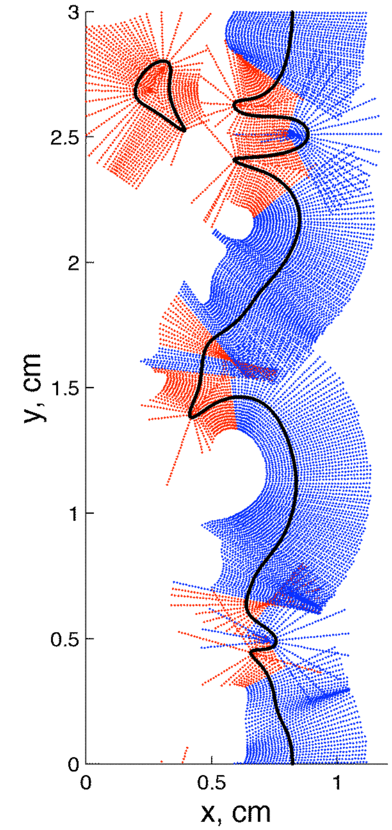
↓

Obtain statistics on the flame feature (Moments, PDFs, conditional statistics etc)

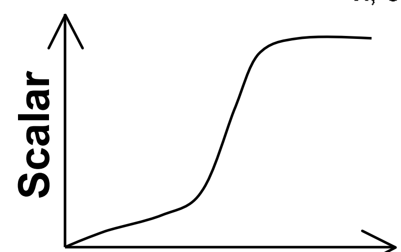
Feature Based Data Analysis

- Isosurface extraction from volume data through triangulation
- Normals extraction from iso-surface vertices
- Data analysis on iso-surface and local normal vector
- Analysis examples:
  - Identify and study flamelet interaction and merging
  - Compute fuel consumption speed.



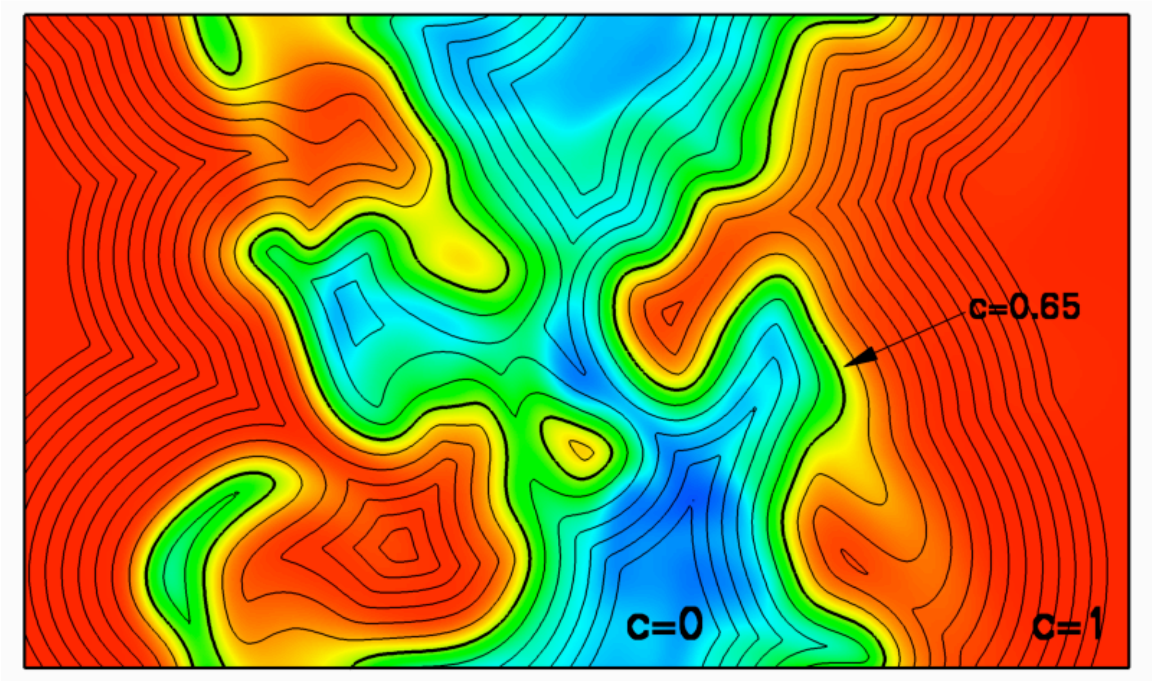


Code developed for performing the analysis in parallel
- Suitable for large data
- Integrated with S3D



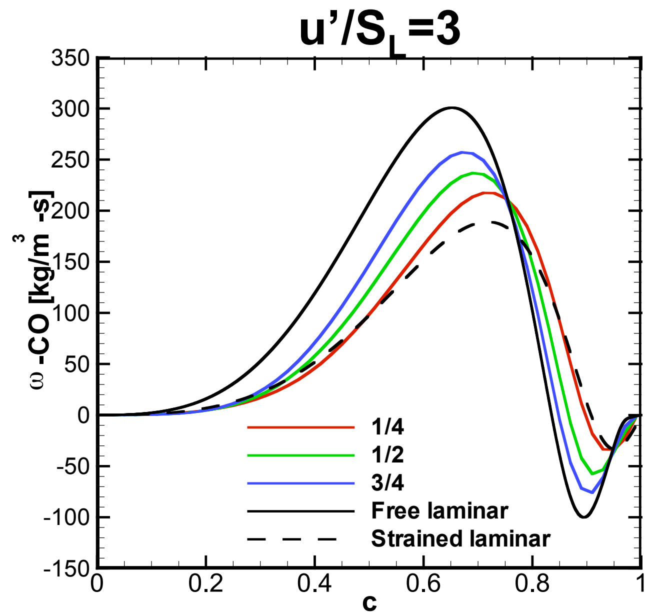
Distance Function Extraction

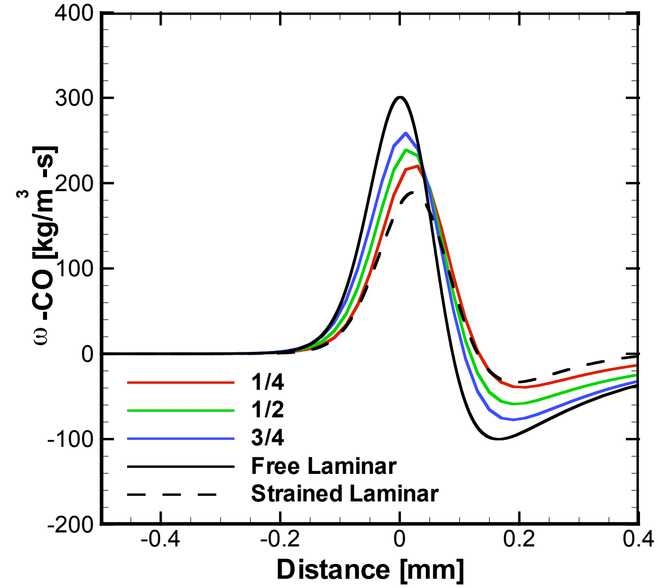
- Define and extract an iso-surface to represent flame
- Compute shortest distance to this surface everywhere in the field by solving the level set equation
  - Surface propagates from the initial condition at uniform speed.

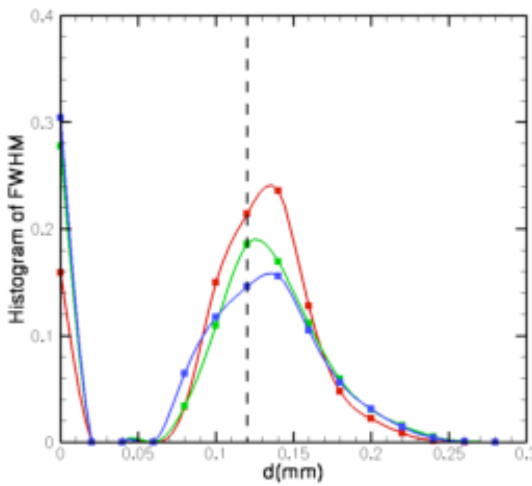


Effect on Reaction Zone

- Did turbulence affect the reaction layer?
- Data conditioned on progress variable and distance from the flame surface.
- Histogram of full width at half maximum (FWHM) of reaction layers obtained through normals analysis.



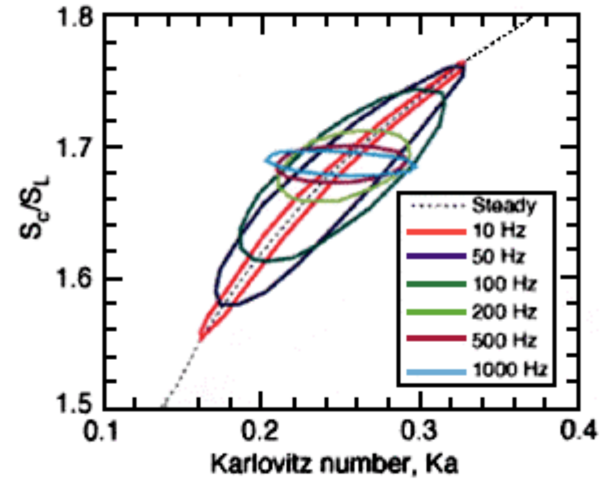


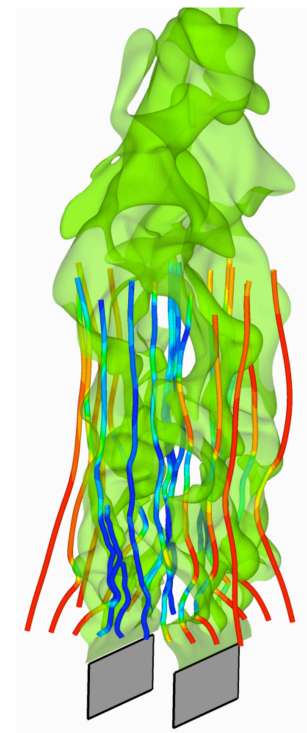


Particle tracking

Work in progress

- Dynamic response of flame to unsteady stretch rate
  - Require time history of flow-flame interaction
- Track history of particles for the duration of simulation
  - Lagrangian fluid particle tracking
  - Iso-surface element tracking
- Parallel algorithm





Summary

- Direct numerical simulations provide unique insight into the physics of turbulent combustion
  - Improved fundamental understanding
  - High fidelity numerical benchmarks
- Leadership systems at NCCS have enabled grand simulations that advance combustion science
- There are challenges in analysis and knowledge extraction from large scale simulation data